Quantum search with resonances

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Abstract

We present a continuous time quantum search algorithm analogous to Grover's. In particular, the optimal search time for this algorithm is proportional to $\sqrt{N}$, where N is the database size. This search algorithm can be implemented using any Hamiltonian with a discrete energy spectrum through excitation of resonances between an initial and the searched state. This algorithm is robust and, as in the case of Grover's, it allows for an error $O(1/\sqrt{N})$ in the determination of the searched state. A discrete time version of this continuous time search algorithm is built, and the connection between the search algorithms with discrete and continuous times is established.

Key words: Quantum computation; Quantum algorithms;
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1 Introduction

In the last twenty years the attention of researchers of several different areas has been attracted towards quantum computation [1,2]. This field of knowledge presents new scientific challenges both from the theoretical and the experimental points of view. Part of the theoretical challenge is to learn how to work with quantum properties to obtain new and more efficient algorithms.

A quantum algorithm can be seen as a definite sequence of unitary transformations acting over a quantum state, in some Hilbert space. Its size is pro-

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portional to the number of elementary unitary transformations of which the algorithm is composed. Concepts like interference phenomena, quantum measurements, resonances, quantum parallelism, amplification techniques, etc., are employed by this new computation science. However, relatively few quantum algorithms were created; among them, Shor's and Grover's [3,4] algorithms are the best known. Shor's algorithm decomposes a number in its prime factors more efficiently than any known classical algorithm. To achieve this it uses quantum parallelism, quantum Fourier transforms, and the properties of quantum measurements. Grover's search algorithm locates a marked item in an unsorted list of N elements in a number of steps proportional to $\sqrt{N}$, instead of $O(N)$ as in the classical case. It performs a unitary transformation of the quantum state which increases the likelihood that the marked state of interest will be measured at the output (amplification technique). It has been proven that there are neither quantum nor classical algorithms that can perform faster such an unstructured search [5].

In this work we present a continuous time quantum search algorithm, which is controlled by a time dependent Hamiltonian. In particular there are not unitary operators that are applied at certain time steps, as in Grover's algorithm. Unlike other authors [6,7] who studied continuous time search algorithms, the most relevant characteristic of our model is the use of quantum resonances, showing explicitly Grover's assertion that his algorithm is a resonance phenomenon [8]. We should remark that a suggestion to employ resonances in quantum computing was made by M. Zak in [9]. The paper is organized as follows. In the next section we develop the continuous time search model. In section 3 we present examples of use of this model for two typical Hamiltonians. Then we show, in section 4, the connection of this continuous time with a discrete time search algorithm. In the last section, we make some concluding remarks.

2   Resonances

The evolution of the wavefunction $|\Psi(t)\rangle$ satisfies the Schrödinger equation,

$$i\frac{\partial|\Psi(t)\rangle}{\partial t} = H \ |\Psi(t)\rangle, \tag{1}$$

where $H = H_0 + V(t)$ and we have taken Planck's constant $\hbar = 1$. Here H_0 is a known nondegenerate time-independent Hamiltonian with a discrete energy spectrum, and $V(t)$ is a time dependent potential that will be defined below. We should point out that the extension to the degenerate case is quite straightforward, as in the case of Grover's algorithm for several equally marked

items.

Let us consider the normalized eigenstates $\{|n\rangle\}$ and eigenvalues $\{\varepsilon_n\}$ for the unperturbed Hamiltonian. These sets can be finite or infinite, depending on the nature of H_0. We now consider a subset $\mathbf{N}$ of $\{|n\rangle\}$ formed by N elements on which we shall apply the search algorithm. We take a known eigenstate $|j\rangle$, with eigenvalue ε_j, as the initial state of the system. This initial state does not belong to the search set $\mathbf{N}$.

Let us call $|s\rangle$ the unknown searched state whose energy ε_s is known. This knowledge is equivalent to 'mark' the searched state in Grover's algorithm. Our task is to find the eigenvector $|s\rangle$ which transition energy from a given initial state $|j\rangle$ is $\omega_{sj} \equiv \varepsilon_j - \varepsilon_s$. We propose the following potential V, which, as it may be easily verified, produces a resonance between the initial and the searched states,

$$V(t) = |p\rangle \langle j| \exp\left(i\omega_{sj}t\right) + |j\rangle \langle p| \exp\left(-i\omega_{sj}t\right), \tag{2}$$

where $|p\rangle \equiv \frac{1}{\sqrt{N}} \sum_{n\in\mathbf{N}} |n\rangle$ is an unitary vector, that can be interpreted as the average of the set of vectors $\mathbf{N}$. This definition assures that the interaction potential V is hermitian, that the transition probabilities from state $|j\rangle$ to any state of the set $\mathbf{N}$ are all equal, $W_{nj} \equiv |\langle n|V(t)|j\rangle|^2 = 1/N$, and finally that the sum of the transition probabilities verifies $\sum_{n\in\mathbf{N}} W_{nj} = 1$.

Let us express $|\Psi(t)\rangle$ as an expansion in the eigenstates $\{|n\rangle\}$ of H_0, $|\Psi(t)\rangle = \sum_m a_m(t) \exp\left(-i\varepsilon_m t\right) |m\rangle$, where the expansion coefficients depend on time. Replacing the above expression of $|\Psi(t)\rangle$ in eq.(1), we obtain the following set of equations for the amplitudes $a_m(t)$

$$\frac{da_n(t)}{dt} = -i \sum_m \langle n|V(t)|m\rangle \, a_m(t) \exp\left(-i\omega_{nm}t\right), \tag{3}$$

where $\omega_{nm} = \varepsilon_m - \varepsilon_n$ are the Bohr frequencies. Combining eqs.(2) and (3), we find,

$$\frac{da_n(t)}{dt} = 0, \tag{4}$$

if $n \notin \mathbf{N}$ and $n \neq j$; and

$$\frac{da_n(t)}{dt} = -\frac{i}{\sqrt{N}} \Bigg\{ (1 - \delta_{nj}) \, a_j(t) \exp\left[+i\left(\omega_{jn} + \omega_{sj}\right) t\right]$$

$$+ \delta_{nj} \sum_{m\in\mathbf{N}} a_m(t) \exp\left[-i\left(\omega_{jm} + \omega_{sj}\right) t\right] \Bigg\}, \tag{5}$$

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if $n \in \mathbf{N}$ or $n = j$.

Before solving numerically the set of eqs.(4) and (5), it is important to understand the qualitative behavior of these equations. Note that there are two time scales involved, a fast scale associated to the Bohr frequencies, and a slow scale associated to the amplitudes $a_n(t)$. Integrating the previous equations in a time interval greater than the fast scale, the most important terms are those that have a very small phase, as the others average to zero. In this approximation the previous set of equations becomes

$$\frac{da_j(t)}{dt} \simeq -\frac{i}{\sqrt{N}} a_s(t) \ , \tag{6}$$

$$\frac{da_s(t)}{dt} = -\frac{i}{\sqrt{N}} a_j(t), \tag{7}$$

$$\frac{da_n(t)}{dt} \simeq 0 \text{ for all } n \neq s, j \ . \tag{8}$$

These equations represent two oscillators that are coupled so that their population probabilities alternate in time. As we notice the coupling is established between the initial and the searched for state. Solving those equations with initial conditions $a_j(0) = 1$, $a_s(0) = 0$ we obtain

$$P_j \simeq \cos^2(\Omega \ t) \ , \tag{9}$$

$$P_s \simeq \sin^2(\Omega \ t) \ , \tag{10}$$

where $\Omega = \frac{1}{\sqrt{N}}$. It is important to notice that this approach is valid only if all the Bohr frequencies verify $\omega_{nm} \gg \Omega$. If we let the system evolve during a time $\tau \equiv \frac{\pi}{2}\sqrt{N}$, and we make a measurement immediately after that, the probability to obtain the searched state is one. For the case that the previous approximations are true, our method behaves qualitatively like Grover's, but the time τ is twice the search time of Grover's algorithm [2]. This difference is not relevant since the resonance potential eq.(2) can be renormalized with a constant factor V_0 as long as it does not invalidate the previous approximations, $\omega_{nm} \gg \Omega$, where now $\Omega = V_0/\sqrt{N}$.

3   Numerical results

We have integrated numerically eqs.(4) and (5) for two Hamiltonians H_0, namely for the quantum harmonic oscillator and for the quantum rotor in 2D. The eigenvalues for these Hamiltonians are $\varepsilon_m = \varepsilon_0(m + \frac{1}{2})$ and $\varepsilon_m = \varepsilon_0 m^2$ respectively. In both cases we take $\varepsilon_0 = 1$ and initial conditions $a_j(0) = 1$, $a_n(0) = 0$, for all $n \neq j$. The calculations were performed using a standard fourth order Runge-Kutta algorithm. Choosing an arbitrary eigenvalue for the energy of the searched state, we follow the dynamics of the set $\mathbf{N}$. We have

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verified, for several values of N, that the most important coupling is between the initial and the searched state, other couplings being negligible, as discussed in the previous section.
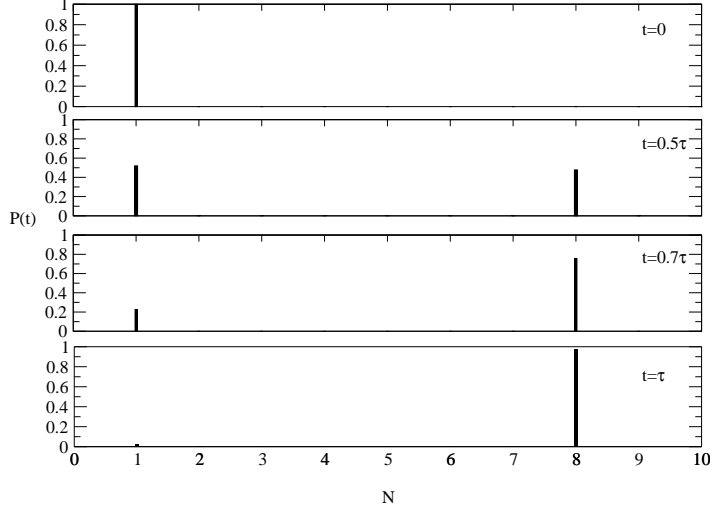

Fig. 1. Time evolution of the probability distribution of the initial and the search set states, for the quantum rotor, for $\mathbf{N} = \{2, ..., 10\}$. The initial state was taken to be $j = 1$, and the searched state $s = 8$. The full line shows the probability of the initial and the searched state. For all the others states of the set the probabilities take negligible values.

The probability distribution of the search set and the initially loaded state are shown for the rotor case in Fig.1. Each panel shows the probability distribution at different times. It is clear that the total probability flows between the initial and the searched states. There is a characteristic time at which the probability of the searched state is maximum and its value is very near one. This time agrees with our theoretical prediction, τ. Fig.2 shows the oscillation of the probability flux between the initial and the searched states as a function of time for the quantum rotor. The temporal evolution was normalized for the characteristic time τ. Fig.3 shows a similar calculation for the harmonic oscillator. Here we have considered three sizes for the data set. Note two remarkable differences between Figs.2 and 3: for the rotor the maximum values of the probabilities are one, while for the harmonic oscillator they are less than one, and decrease with time. Furthermore, while for the rotor the maxima are located in agreement with the theoretical prediction, for the harmonic oscillator the maxima show an increasing shift to the right of the predicted values as the search algorithm evolves.

The differences between the two Hamiltonians mentioned above are due to the properties of their respective energy spectra: while the energy eigenvalues of

the rotor increase quadratically with the quantum number, for the harmonic oscillator they increase linearly. Consequently, the condition $\Omega << \omega_{nm}$, is better satisfied for the spectrum of the rotor than for the harmonic oscillator. As a consequence the agreement with the theoretical approximation is worse in this last case. However, as $\Omega = \frac{1}{\sqrt{N}}$, if the size of the data set is increased, the agreement for the harmonic oscillator with the behavior predicted by eq.(10) is much improved, as shown in Fig.3. Increasing N leads to a decrease in the relative distance between the energy spectrum values of H_0, allowing for a better resolution. In general, for a given Hamiltonian H_0 with a discrete energy spectrum, the improvement obtained increasing N becomes negligible after some saturation value. Above this saturation value the algorithm presented here, has the same characteristics as Grover's algorithm.
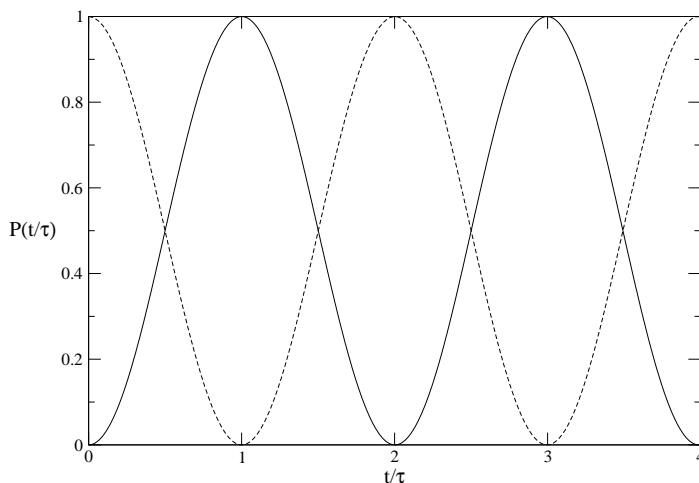

Fig. 2. Probability distribution for the initial (dashed line) and the searched (full line) states as a function of time for the quantum rotor H_0 in the case of a data set of size $N = 20$

The proportionality between the characteristic time τ and $\sqrt{N}$ for the rotor and the harmonic oscillator, is verified in Fig.4.

Taking N greater than its saturation value, one can test the robustness of this search algorithm with respect to imprecisions in the eigenvalue of the searched state. Let us replace ω_{sj} by $\widetilde{\omega}_{sj} \equiv \omega_{sj} + \delta$ in eqs.(5), where we take δ smaller than Ω .
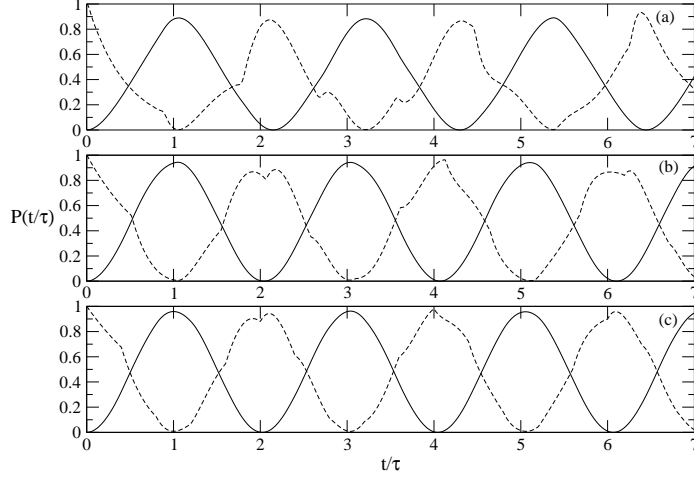
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Fig. 3. Probability distribution for the harmonic oscillator H_0 as a function of time. The dashed line corresponds to the initial state and the full line to the searched state. The size of the searched set are: (a) $N = 20$, (b) $N = 60$, (c) $N = 100$.
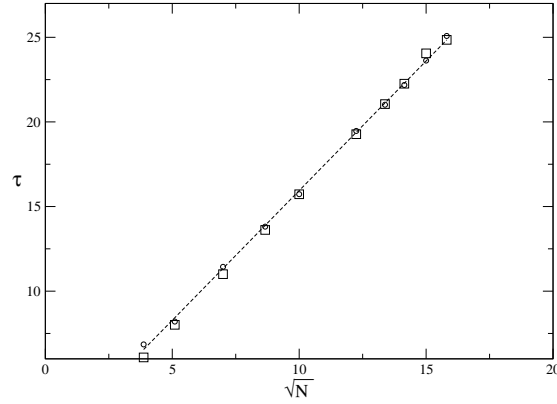

Fig. 4. Time τ at which the probability of the searched state is maximum as a function of the square root of the dimension of the search set. Squares correspond to the harmonic oscillator, and circles to the rotor.

Within the this approximation the probability of the searched state evaluated in $t = \tau$ is,

$$P_s(N, \delta) = \left[\frac{\sin \left(\frac{\pi}{2} \sqrt{1 + \frac{\delta^2 N}{4}} \right)}{\sqrt{1 + \frac{\delta^2 N}{4}}} \right]^2 . \tag{11}$$

We define the resonance width Δ, as the value of δ for which the probability of the searched state falls to half of the value for $\delta = 0$.
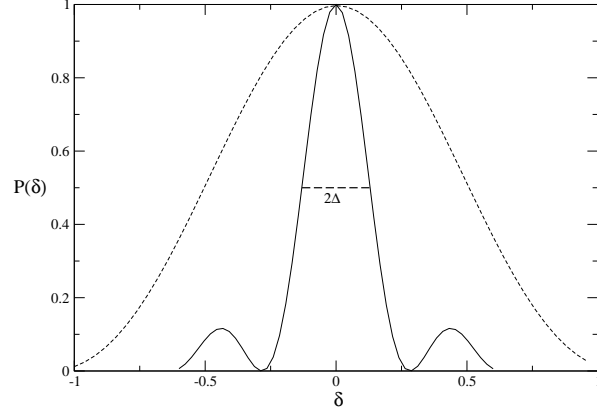
Fig. 5. Probability to find the searched state as a function of the energy error δ, for the rotor, with $N = 10$ (dashed line) and $N = 100$ (full line). Δ is the width of the resonance.

The calculation of the probability of the searched state as a function of δ is presented in Fig.5. It can be observed that the curves are in agreement with eq.(11), showing a symmetrical behavior about $\delta = 0$ and a sharpness that depends on N. For small δ the probability of the searched state remains large enough. Then, we deduce that a small error in ω_{sj} does not affect drastically the search algorithm.
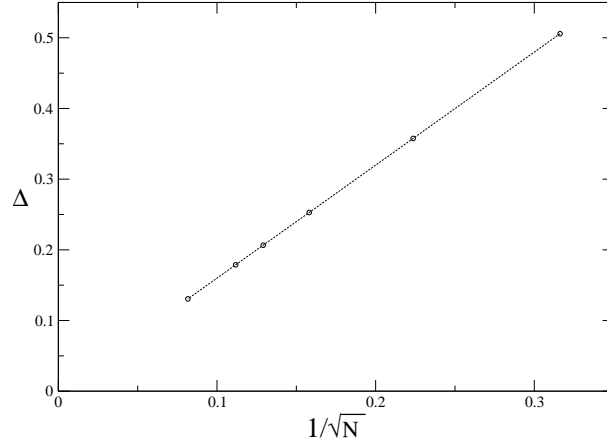

Fig. 6. Resonance width as a function of $1/\sqrt{N}$. The points are results of the numerical calculation. The dashed line corresponds to the linear regression of the data.

The dependence of the resonance width with N is presented in Fig. 6. The numerical calculation fits with a hyperbola defined by $\Delta\sqrt{N} \simeq 1.599$. This result is in agreement with eq.(11) when $P_s(N,\delta) \simeq \frac{1}{2}$ with $\delta = \Delta$.

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4   Connection with a discrete time search algorithm

We now build a discrete version of the continuous time algorithm developed in the previous sections. Note that the time τ can be expressed by $\tau = \pi/(2\Omega) = \sqrt{N}\omega_{sj}T/4$, where $T = 2\pi/\omega_{sj}$ is the period of interaction potential, eq.(2). Then one can use Floquet's theory [10] to obtain the matrix of the Floquet evolution operator $U_F = U_F(T)$. If one defines an unitary evolution operator $U_D \equiv (U_F)^{\frac{\omega_{sj}}{4}}$, the searched state is obtained by applying U_D $O(\sqrt{N})$ times to the initial state. If $\omega_{sj}/4$ is not an integer number, we round it to the nearest integer in the definition of U_D.

To construct the Floquet operator, we must look for the amplitudes of the Floquet states that are also solutions of the eqs.(5). These amplitudes have the form

$$a_m(t) = \exp\left(-i(\lambda - \varepsilon_m)t\right) \langle m |\ \phi_\lambda(t)\rangle, \tag{12}$$

where $|\phi_\lambda(t)\rangle = |\phi_\lambda(t + T)\rangle$ is the λth Floquet state and λ is the corresponding Floquet parameter. As $|\phi_\lambda(t)\rangle$ is periodic, it can be expanded as a Fourier series

$$\langle m |\ \phi_\lambda(t)\rangle = \sum_{k=-\infty}^{\infty} A_k(m, \lambda) \exp\left(il\omega_{sj}t\right). \tag{13}$$

Using the eqs (12,13) in eq.(5) we obtain set of equations for the parameter λ and for the amplitudes A_k

$$(-\lambda + \varepsilon_j + k\omega_{sj})\, A_k(j, \lambda) = -\frac{1}{\sqrt{N}} \sum_{m=1}^{N} A_{k+1}(m, \lambda), \tag{14}$$

$$(-\lambda + \varepsilon_n + k\omega_{sj})\, A_k(n, \lambda) = -\frac{1}{\sqrt{N}} A_{k-1}(j, \lambda), \text{ for all } n \in \mathbf{N}. \tag{15}$$

Replacing A_{k+1} from eq. (15) into eq. (14), the characteristic equation for λ is obtained

$$xN = \sum_{m=1}^{N} \frac{1}{x + \omega_{sm}}, \tag{16}$$

where $x \equiv -\lambda + \varepsilon_j + k\omega_{sj}$. This equation has $N + 1$ solutions for both x and λ. Note that the indetermination in λ introduced by the term $k\omega_{sj}$ is superfluous since the Floquet evolution operator is evaluated at $t = T$ and therefore $\exp(-ik\omega_{sj}T) = 1$. Once we have the values for λ we obtain the Fourier coef-

ficients $A_k(m, \lambda)$ and, using eq.(13), $\langle m | \phi_\lambda(t) \rangle$.

The Floquet matrix has the form

$$(U_F)_{mn}(T) = \sum_\lambda \exp(-i\lambda T) \langle n | \phi_\lambda(0) \rangle \langle \phi_\lambda(0) | m \rangle, \qquad (17)$$

and, therefore,

$$(U_D)_{mn}(T_0) = \sum_\lambda \exp(-i\lambda T_0) \langle n | \phi_\lambda(0) \rangle \langle \phi_\lambda(0) | m \rangle, \qquad (18)$$

where $T_0 = \omega_{sj} T/4$. Interpreting U_D as a rotation operation with angle λT_0, its application to the initial state $O(\sqrt{N})$ times, maximizes the probability to find the searched state. Then for any H_0 one can build a discrete time algorithm to perform the search.

5   Conclusions

We have developed a new insight in generating a continuous time quantum search algorithm using a characteristic of quantum mechanics, quantum resonances. This algorithm behaves like Grover's algorithm; in particular the optimal search time is proportional to the square root of the size of the search set, $\sqrt{N}$, and the probability to find the searched state oscillates periodically in time. The efficiency of this algorithm depends on the spectral density of the Hamiltonian H_0. A bigger separation between the energy levels maximizes the probability of the searched state and allows for a better precision. For any Hamiltonian with discrete energy spectrum, independently of its spectral density, this algorithm can be implemented taking a large enough search set.

The algorithm was shown to be robust when the energy of the searched state has some imprecision. However the improvement in the accuracy of the search by increasing N, and the error margin are bounded by the relation $\Delta\sqrt{N} = $ constant. This means that for a large N it demands a good precision in the eigenvalue of the searched state. Noting that Δ is an energy variation, and $\sqrt{N}$ is the time needed for the measurement, the previous relation is simply the Heisenberg uncertainty principle.

We have found a simple way to build a discrete time algorithm on the basis of our continuous time search algorithm, which strongly suggests the equivalence between search algorithms with discrete and continuous time.

It has been recently shown that Grover's algorithm may not be directly applicable to search in a physical database[7]. Indeed, it has also been pointed

out that it would be neither technologically nor economically reasonable to build database search engines basen on Grover's search algorithm[11]. Similar questions might be raised about the algorithms presented here.

Regarding the implementation of these algorithms, we note that the quantum kicked rotor has been experimentally realized using ultra-cold atom traps and some experiments have focused on the resonant case [12]. Furthermore, we have recently shown that the discrete quantum random walk on the line has the same dynamics as the kicked rotor in resonance [13,14]. Several systems have been proposed as candidates to implement quantum random walks [15,16,17,18,19]. When these devices are constructed, they may be employed to simulate the search algorithms proposed here.

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